Software

Unintentional fragment handling

Overview

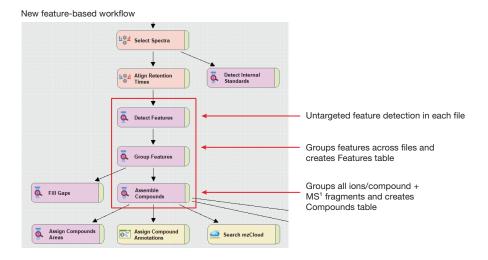
Unintentional fragmentation, also known as transmission-related fragmentation (which can include adducts, dimers, isotopes, and in-source fragmentation), occurs during the mass spectrometry process, where ions may break apart as they pass through the instrument. These additional ion signals complicate data interpretation and reduce reliability unless handled correctly. Thermo Scientific[™] Compound Discoverer[™] software 3.4 introduces a new feature-based workflow with advanced transmission-related fragment handling capabilities, automating the identification and reduction of transmission-related fragments to enhance data clarity and accuracy.

Method

Compound Discoverer software matches transmission-related fragments with the precursor by correlating fragmentation data from the MS² scan with peaks that are detected in the full scan. To increase confidence, Compound Discoverer software also makes use of the low collision energy information that is available from the mzCloud[™] spectral library. For compounds that can be matched to the data based on authentic standards in mzCloud, Compound Discoverer software automatically retrieves the scan with the lowest collision energy that is available in the spectral library and uses this information to confirm the association between a suspected transmission-related fragment and the precursor.

Key features

- 1. Automated fragment identification: The new algorithm in Compound Discoverer software 3.4 automatically identifies transmission-related fragments, which were previously managed manually, and reduces them into a single compound. This feature simplifies your analysis and ensures that data processing is more efficient and less prone to human error.
- 2. Comprehensive data reduction: The automation of transmission-related fragment handling reduces the need for manual intervention, speeding up the data processing workflow so you can focus on data interpretation and analysis.
- **3.** Enhanced data clarity: By eliminating chemical noise and artifacts, the software provides a clearer and more accurate representation of the actual compounds present in the sample. This leads to more reliable results in your metabolomics research.
- 4. Confident purity assessment: There is so much stuff in complicated samples, even with best separations and methods you may inevitably have coelutions. The new MS² purity column in the compounds table provides a measurable degree of chimerism within an RT window for each compound, helping you build confidence in the clarity of your data.



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New feature-based workflow | Compounds table with Features sub-table

	Comp	ounds Compo	ounds per Fil	e Features	Features per File	Internal St	andards	Internal Stand	ards per File	mzCloud	i Results	LipidSe	arch Re	sults	ChemSpic	ler Results Inpu	t Files	Study Inform
	7	Name Formula		Α	Annot. Source 🛨		Calc. MW	m/z	Reference Ion	RT [min]	[min] Area (Max.]		 Polarity MS2 		AS2 Purity (%] Peak Rating (Ma	x.) Gro	up Areas 🛨
1	-	Citric acid C6 H8 O7					192.02685 191.0195		[M-H]-1	2.465 205359202		2021	+/-		10	0	9.5 1.0	5e9 2.05e9
	-	α-Lactose	C12 H22 O1	1		-0.14	342.11616	685.23962	[2M+H]+1	1.337	587534	8199	/-		10	0	9.5 4.6	3e8 5.88e8
\odot	Hide R	elated Tables																
Sn	ucture	Proposals Compounds per File Predict			Compositions	Features mzCloud		esults Lipio	iSearch Results	Chem	ChemSpider Results		Mass List Searc		ch Results			
	P	lon	Charge	Adduct Feature	 Molecular Weig 	ht m/z	RT (min] FWHM [mir] Area (Max.)	 Intensi 	ty (Max.)	# MI (Ma	x.) MS	2 MS	2 Purity [%]	Peak Rating (Max.)	Peak R	ating 🛨 (
1	-12	[M-H]-1	-1	Yes	192.0268	1 191.019	53 2.463	0.07	2 205359202	1 39	8788672		3		100	9.5	8.4	9.5
2	-12	[2M+Na]+1	1	Yes	192.0269	9 407.043	19 2.464	0.07	177434530) 3	5446957		4		97	8.9	8.9	8.4
3	-12	[M+K]+1	1	Yes	192.0269	8 230.990	14 2.448	0.08	4 3265081	6	5585975		3		89	9.5	8.4	9.5
4	-12	[M+NH4]+1	1	Yes	192.0270	3 210.060	85 2.465	0.07	2101925	5	3808026		3		100	8.4	8.4	8.4
5	-12	[2M+H]+1	1	No.	102.027	0 205 061	2.464	0.05	7 882739	1	2363702		2		100	8.9	8.9	8.9
6	-12	[2M-H]-1	-	+ve an	d –ve mo	de io	ns 2.45	0.06	4 666965	4	1686510		2		100	9.1	9.1	7.8
7	-12	[M+Na]+1	1	res	192.0270	0 215.010	2.48	0.08	30179990	5 4	5281828		3		100	9.5	9.5	8.4
8	-12	[M+H]+1	1	Yes	192.0269	4 193.034	21 2.463	0.06	5 9167662	4 1	9324864		3		100	9.5	9.5	8.4
9	-12	[X-e]+1	1	No	147.0293	6 147.028	81 2.460	0.06	5 10953048	3 2	4271686		3		99	9.5	9.5	9.5
1	0 👳	[X-e]+1	-	MS	¹ Transm	ission	-relat	ed	5 8375592	8 1	8422246		3		99	9.5	8.4	9.5
1	1 👳	[X-e]+1	1						5 4592057	5	9881318		2		99	8.4	8.4	8.4
1	2 👳	[X-e]+1	1		Iragi	nents			1164577	5	2637905		2		98	9.5	9.5	8.9

New columns in the Compounds table

C	ompo	ounds Com	pounds per File Feature	Features per File	Internal Standards	Internal Sta	ndards per f	File mzClo	oud Results	LipidSearcl	n Results C	hemSpide	r Result	s Input Files	Study	/ Information	Statistical Me	thods	
P		Comments	Name	Formula	Annot. Source 🛨	Annot. ∆Ma	Calc. MW	m/z	Reference lor	n RT (min)	Area (Max.)	• Polarit	MS2	MS2 Purity [%]	Group	Areas 🛨 Pe	ak Rating (Max.)	Peak Rat	ting [
1	-	check	Citric acid	C6 H8 O7		-0.79	192.02685	191.01953	[M-H]-1	2.465	205359202	1 +/-		100	1.05e9	2.05e9	9.5	8.4	9.5
2	-		α-Lactose	C12 H22 O11		-0.14	342.11616	685.23962	[2M+H]+1	1.337	58753819	9 +/-		100	4.63e8	5.88e8	9.5	9.5	8.9
3	-	interesting!	3-Methyl-1,3-benzothiazo	-: C8 H8 N S		1.10	150.03791	133.03462	[M+H-H2O]+	14.532	41337361	3 +			4.04e8	4.1368	5.7	4.6	5.7
4	-		D-Glucose	C6 H12 O6		-0.16	180.06336	215.03276	[M+CI]-1	1.280	40579343	6 -		100	1.92e8	4.05e8	10.0	8.4	10.1
5	-		Acetyl-L-carnitine	C9 H17 N O4		-1.57	203.11544	204.12272	[M+H]+1	2.027	31015928	7 +		86	1.35e8	3.10e8	9.5	9.5	8.4
6	-		α,α-Trehalose	C12 H22 O11		-0.24	342.11613	387.11412	[M+FA-H]-1	1.552	25802759	8 +/-		100	2.32e8	2.58e8	8.9	8.4	8.9
7	-		Creatine	C4 H9 N3 O2		-0.18	131.06945	132.07673	[M+H]+1	1.395	23619131	2 +		100	1.43e8	2.35e8	10.0	10.0	9.5
8	-			C28 H47 CI O15 P2		1.31	720.20882	719.20154	[M-H]-1	1.311	21096012	7 -		100	1.98e8	2.11e8	8.9	8.9	7.8
9	-		Choline Alfoscerate	C8 H20 N O6 P		0.38	257.10292	258.11020	[M+H]+1	1.291	20308980	0 +		100	1.96e8	2.03e8	9.5	8.4	9.5
10	-		Lauryldiethanolamine	C16 H35 N O2		-0.14	273.26674	274.27402	[M+H]+1	10.406	18173967	8 +			1.81e8	1.82e8	9.5	9.5	8.4
11	-12			C2 H5 N3 O3 P2		-3.64	180.97995	163.97668	[M+H-H2O]+	14.883	17245157	• 0		80	1.72e8	1.61e8	5.7	5.7	5.7
12	-i=		trans-Aconitic acid	C6 H6 O6		-0.23	174.01640	175.02367	[M+H]+1	2.461	15868672	0 +/-		100	6.93e7	1.59e8	8.4	8.4	8.4

MS² Purity = <u>intensity of target mass centroid</u> total intensity of all centroids within isolation window x 100

Benefits

- Efficiency: Automated processes save time and reduce the workload on researchers.
- Accuracy: Improved fragment handling ensures more precise identification of compounds.
- **Data quality:** Reduction of chemical noise and artifacts leads to higher quality data and more reliable results.

Conclusion

The transmission-related fragment handling capabilities in Compound Discoverer software 3.4 streamline the data processing workflow, providing researchers with a powerful tool to achieve more accurate and efficient metabolomics analysis.

Learn more at thermofisher.com/compounddiscoverer

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